

Event Generators for Simulating Heavy Ion Interactions of Interest in Evaluating Risks in Human Spaceflight¹

Lawrence S. Pinsky
Physics Department
University of Houston
4800 Calhoun Blvd.
Houston, TX 77204-5005
713-743-3552
pinsky@uh.edu

Victor Andersen, Anton Empl, Kerry Lee, Georgi Smirnov and Neal Zapp
Physics Department
University of Houston
4800 Calhoun Blvd.
Houston, TX 77204-5005, USA

Alfredo Ferrari, Katerina Tsoulou, Stefan Roesler and Vasilis Vlachoudis
CERN
CH-1211
Geneva, Switzerland

Giuseppe Battistoni, Mauro Campanella, Francesco Cerutti, Ettore Gadioli, Maria-Vittoria Garzelli, Silvia Muraro, Tiziana Rancati and Paola Sala
INFN and University of Milan,
Via Celoria 16
20133 Milan, Italy

Francesca Ballarini, Andrea Ottolenghi, Vincenzo Parini and Domenico Scannicchio
INFN and University of Pavia
Via Bassi 6
27100 Pavia, Italy

Massimo Carboni and Maurizio Pelliccioni
Laboratori Nazionali di Frascati
INFN, Frascati
Via E. Fermi 40
00044 Frascati, Italy

Thomas L. Wilson
Mail Code SR
NASA/JSC
Houston, TX, 77058, USA

Johannes Ranft
Physics Department
Siegen University
D-57068 Siegen, Germany

Alberto Fasso'
Stanford Linear Accelerator Center
2575 Sand Hill Road
Menlo Park, CA 94025

¹ 0-7803-8155-6/04/\$17.00©2004 IEEE

Abstract— Simulating the Space Radiation environment with Monte Carlo Codes, such as FLUKA, requires the ability to model the interactions of heavy ions as they penetrate spacecraft and crew member's bodies. Monte-Carlo-type transport codes use total interaction cross sections to determine probabilistically when a particular type of interaction has occurred. Then, at that point, a distinct *event generator* is employed to determine separately the results of that interaction. The space radiation environment contains a full spectrum of radiation types, including relativistic nuclei, which are the most important component for the evaluation of crew doses. Interactions between incident protons with target nuclei in the spacecraft materials and crew member's bodies are well understood. However, the situation is substantially less comfortable for incident heavier nuclei (heavy ions). We have been engaged in developing several related heavy ion interaction models based on a Quantum Molecular Dynamics-type approach for energies up through about 5 GeV per nucleon (GeV/A) as part of a NASA Consortium that includes a parallel program of cross section measurements to guide and verify this code development.

Table of Contents

1. Introduction	2
2. The RQMD Event Generator	3
3. Improved Event Generators	5
4. Conclusions.....	6
	References
	6
Biography	6

1. Introduction

The space radiation environment is complex and impossible to re-create in the laboratory. While individual components can be provided in ground-level experiments it is beyond the current technology to reproduce the combined spectra of all the constituents. As such, we are constrained to rely on computer simulations to predict the nature of the radiation field behind various shielding scenarios that are exposed to the space radiation environment. One of the computational techniques employed is the so-called Monte-Carlo transport method. Based on a representation of the geometry and composition of the shielding materials, individual incident particles are transported and interactions are modeled probabilistically based on the known cross sections for them within each particular kind of medium. The computer codes themselves generally split the calculations into two distinct parts, one of which uses the relevant total cross section to ask if any interaction occurs, and the second, called an *event generator* is then employed to simulate the details of the interaction whenever one takes place. Typical uses call for the

simulation of very large numbers of incident particles in order to reduce the statistical uncertainty in the final predictions. Of course, statistics cannot overcome any weaknesses in the accuracy of the basic event generators.

Excellent event generators exist for most kinds of interactions, such as those which occur when electrons or photons are being propagated, or when individual nuclear particles such as protons, neutrons or pions are involved. However, the event generators for nucleus-nucleus collisions, especially in the energy regime from the threshold for such interactions starting around a few MeV/A up through about 5 GeV/A are on much less firm footing. Part of the reason for this is the wide range of physics that occurs in this part of the energy spectrum and the involvement of the details of nuclear structure. At much higher energies, the situation actually becomes easier to model as far as the aspects of interest in predicting dose-type effects are concerned, and again adequate event generators for those interactions also exist.

In order to address this need, NASA has formed two related Consortia, one devoted to the modeling necessary to produce these event generators, and the other charged with measuring the cross sections necessary to guide and validate the models.[1] One of the reasons that the existing models are not as far along as those for other types of interactions is indeed the lack of data of the kind that are necessary to fine-tune and gain confidence in the models. It is not possible to make a detailed enough series of measurements with all projectile-target-energy combinations to use empirical models that simply fit the data. Rather, one must develop physics-based models and gain sufficient confidence that they do represent the fundamental physics processes correctly enough to be valid within reasonable limits when they are called upon to simulate interactions for which we have no data.

To that end, we have selected the RQMD models of Sorge as a starting point.[2] One of the most successful approaches to modeling the interactions of individual particles with nuclei has been the Intra-Nuclear Cascade (INC) technique.[3] In this model the target nucleus is represented as a collection of protons and neutrons with appropriate energy distributions held in a global nuclear field. The incident particle is then transported through this representation probabilistically using the free-particle interaction cross sections with the protons and neutrons, and employing a separate model for the interaction of the particle with the nuclear field. In these models, a constant mean field is assumed throughout. This “mean-field” approximation works well when the incident particle is a proton and the target is a heavy nucleus. However, when the projectile and target are both composite nuclei, this mean-field approximation is likely to be less accurate in its representation of the situation.

Chemists have faced a similar problem in modeling molecular dynamics. When a molecule is isolated, its structure is typically easily modeled. However, in the proximity of other molecules, the atoms in the first molecule begin to feel the separate influence of the charges of other nearby atoms in adjacent molecules, distorting the real field that they see. To overcome this, an iterative extension called QMD (Quantum Molecular Dynamics) was introduced.[4] That approach actually recalculates the field at the end of each small time step felt by every particle due to the presence of all nearby atoms, and not just the ones in its own molecule. RQMD is an adaptation of that technique to the world of nuclear interactions. As in the case of the INC models, the nuclei are represented by collections of protons and neutrons that are being held together by their own mutual nuclear field. The difference is that instead of using the mean field method, RQMD follows the lead of the chemists and recalculates the field at each time step.

We have a version of the FLUKA transport code that has had a modified version of the RQMD code embedded in it to handle the nucleus-nucleus collisions up to an energy of 5 GeV/A.[5] To cover energies above this value we embed the DPMJET III event generator.[6] We are also working on an extension to an additional event generator to be employed at energies below 100 MeV/A based on the Boltzmann Master Equation approach.[7] The present paper will focus on our progress and some of our results on the RQMD event generator and our efforts to come up with an improved version as well as an alternate event generator using a somewhat modified approach.

2. The RQMD Event Generator

The version of RQMD that is included in the present release of FLUKA is a modified version of the well known code developed by Sorge.[2] This code has an option to run in an INC-like mode to reduce computation time in instances where the full accuracy is not required. The fundamental code has not been changed, but some modifications to the outputs in the form of energy re-normalizations were required to insure absolute energy conservation, which is an essential requirement of the overlying FLUKA transport code.

The RQMD code itself can in principle reach the final state directly, but allowing it to do so would be prohibitive in execution time. In addition, the approximations used to recalculate the nuclear field, which are also necessary to keep execution time within reason, do not give a particularly impressive result for representing some of the correct details of the nuclear structure. As such, the strategy is to allow the code to evolve the interaction to some intermediate point where essentially all of the hard

collisions by the constituent particles are over, and then to halt the evolution. A separate routine then surveys this interim state and attempts to collect the nucleons into fragments based on their proximity in phase space. Lastly, the remaining particles are placed in the final state event generator output buffer, and the trial fragments identified in the previous step are run through a pre-equilibrium processor and an evaporation code that allows them to de-excite into a surviving fragment, which may have boiled-off some of its original constituents in the evaporation process. The selection of the exact point in the RQMD evolution at which the process is turned over to these final state handlers is a potentially tunable parameter that can be used as data become available to attempt to optimize the fit.

Figures 1 - 6 show some results from the RQMD event generator as it is exercised within the FLUKA code. These fluence plots (number of particles cm^{-2}) were all prepared to aid in the planning for proposed future measurements at the Alternating Gradient Synchrotron (AGS) at the Brookhaven National Laboratory on Long Island. They all depict the laboratory scattering angles in annular angle bins of one degree for protons above a kinetic energy of 100 MeV in the laboratory, for all charged pions above 50 MeV in the laboratory and for all light ions (Deuterons through Boron) above 100 MeV/A. The ordinates are all normalized to the yields from a 1 kHz beam incident on a one interaction length target.

All of the figures show a similar behavior with a proton distribution peaking near zero (note that the integration over the annular area of each angle bin distorts the areal density distribution of the tracks, which is centrally peaked). The pion scattering angle distribution rises from low values at small angles, becoming comparable to or exceeding the proton fluences between 15 and 20 degrees.

One of the important differences in the calculations for 5 GeV/A incident projectiles with respect to similar 3 GeV/A interactions is the relative height of the pion distributions at these larger angles.

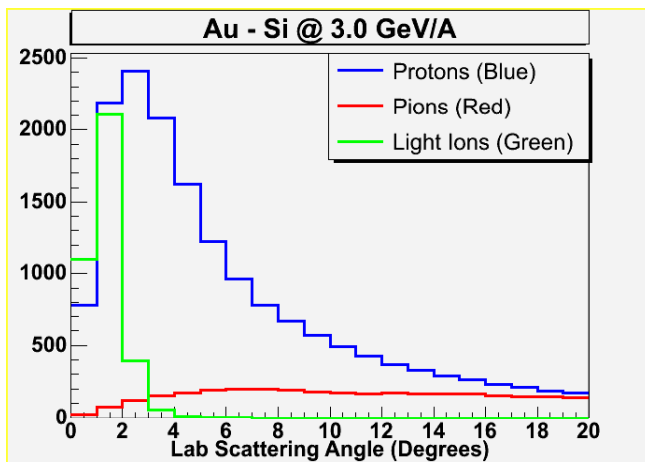


Figure 1 – Laboratory Scattering Angle Distributions for protons, pions and light ions (D-B) per second in one degree annular bins from a 1 kHz 3.0 GeV/A Gold (Au) beam incident on a one interaction length thick Silicon (Si) target.

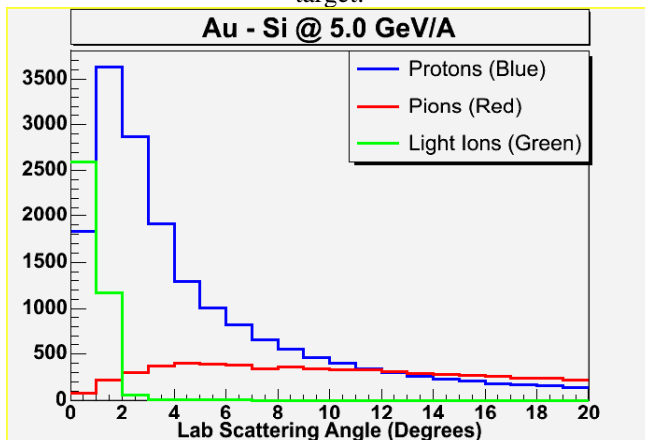


Figure 2 – This should be compared with Figure 1. It shows the Laboratory Scattering Angle Distributions for protons, pions and light ions (D-B) per second in one degree annular bins from a 1 kHz 5.0 GeV/A Gold (Au) beam incident on a one interaction length thick Silicon (Si) target. Note the dominance of the pions starting at about 13 degrees.

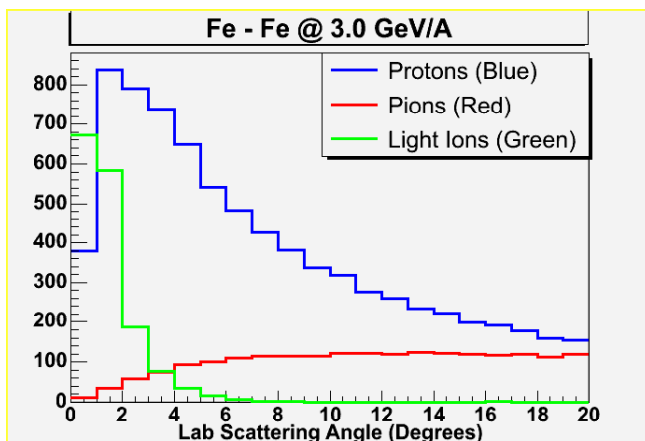


Figure 3 – Laboratory Scattering Angle Distributions for protons, pions and light ions (D-B) per second in one degree annular bins from a 1 kHz 3.0 GeV/A Iron (Fe) beam incident on a one interaction length thick Iron (Fe) target. Note the greater angular range for the light ions and the flatter proton distribution as compared with the Au-Si plots in Figures 1 and 2.

In comparing these plots it is important to consider the absolute values of the fluences as a function of both energy and the size of the projectile and target. Generally, the fluences are bivariate and scale with both of these parameters. The plots tend to include mostly the contributions from the projectiles only, as the fragments from the target typically have laboratory kinetic energies below the cutoffs used here. There are differences in the plots in terms of the relative ratios of protons to pions and in

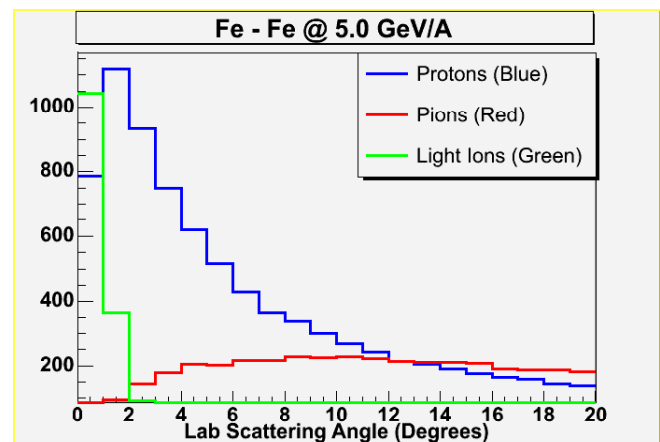


Figure 4 – Laboratory Scattering Angle Distributions for protons, pions and light ions (D-B) per second in one degree annular bins from a 1 kHz 5.0 GeV/A Iron (Fe) beam incident on a one interaction length thick Iron (Fe) target. Note the similar shape, but at significantly lower fluences than in the Au-Si case at 5.0 GeV/A in Figure 2.

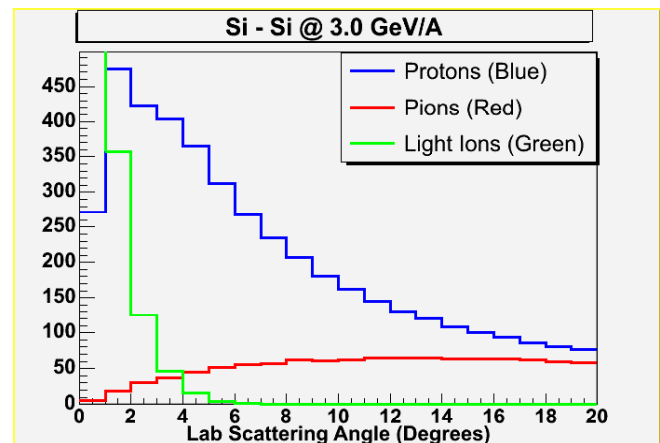


Figure 5 – Laboratory Scattering Angle Distributions for protons, pions and light ions (D-B) per second in one degree annular bins from a 1 kHz **3.0 GeV/A Silicon (Si)** beam incident on a one interaction length thick Silicon (**Si**) target. Compare this with the plot in Figure 3, noting the similarity in the shape of the distributions but the difference in the absolute magnitudes of the fluences. Also note the differences in the light ion fluences in the central most angle bin.

the angular distributions of the light ions, especially at the more central angle bins. Also, in Figures 1 and 6, the collision is between decidedly asymmetrical projectile and target masses. These plots show some of the differences one can expect from asymmetrical situations such as given here.

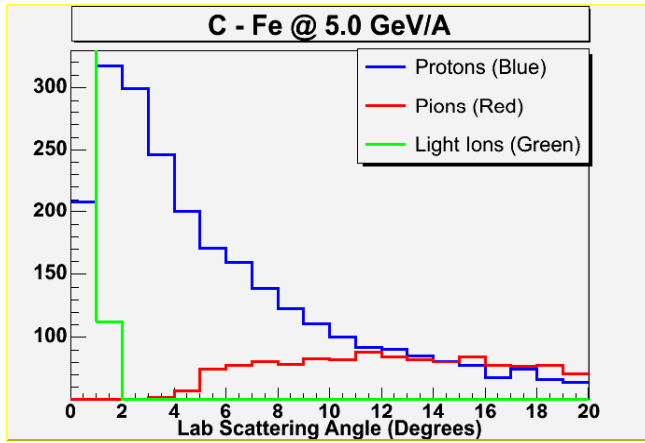


Figure 6 – Laboratory Scattering Angle Distributions for protons, pions and light ions (D-B) per second in one degree annular bins from a 1 kHz **5.0 GeV/A Carbon (C)** beam incident on a one interaction length thick Silicon (**Fe**) target. Note that this represents a case of very non-symmetric collision participants, and the effects are noticeable as compared to the more symmetric participants in Figures 2-5.

3. Improved Event Generators

We have taken three paths towards improving this existing RQMD event generator. The first is to tune up the supporting software that does the fragment collecting after the event generator evolution is stopped and the evaporation of those fragments occurs. The second is to delve into the core of the event generator to try and clean up the approximations that were made by the original author and lead to the energy non-conservation behavior. Both of these two approaches keep the same basic code in place. The third path is to develop an entirely parallel

approach, termed the Hamiltonian Molecular Dynamics model (HMD) that focuses on the details of the needed relativistic transformations internally within the evolution processor. None of these efforts is ready to produce results for comparison with the existing generator or with data, but hopefully by the time of the oral presentation, some preliminary results will be forthcoming. We limit ourselves here to providing a brief description of the work on this third path.

The HMD model is based on the concept of the constrained Hamiltonian as introduced by Dirac,[8] and developed by Todorov and Komar.[9, 10] Effective nucleon-nucleon potentials are given in a non-relativistic form (e.g. as a function of 3-distance). Clearly the challenge is to cast nucleon (and thus nuclear) equations of motion which are nevertheless manifestly covariant. In moving from a Wigner-picture 6-N dimensional quasi-phase space to Minkowski space, we see that the number of degrees of freedom increase by 2N. Thus, 2N equations of constraint allow us to define the world-lines for each particle in the system uniquely.

Potentials are included by making the philosophical approximation that the effect of the potentials on system trajectory is to alter the transverse momentum distributions, so that the argument of the potential functional is transformed to the transverse 4-distance, making the potentials by definition Poincaré scalars. Alternatively, one can also show by solution of the system Hamiltonian characteristic equations that this choice of argument is the single value allowing the Hamiltonian to reach the local extremum value required by the variational principle.

Working according to the constrained Hamiltonian formalism, the Hamiltonian is written as a linear combination of the (scalar) constraint equations, the coefficients being elements from the inverse of the Poisson matrix. We believe that the energy conservation issues realized by previous authors are overcome via a tedious, but necessary individual calculation and combination of single-particle Hamiltonians and correlation (potentials and Hilbert coherence) energies. This has been shown correct for a limited range of systems, and a more general validation of this contention is currently ongoing.[2, 11, 12, 13]

In its current form, this model makes use of the free-particle nucleon-nucleon elastic cross sections to describe successive particle collisions, with no inclusion of inelastic channel probabilities. We recognize that this is insufficient for a full description of the system, both in terms of the inclusion of inelastic reactions, and the alteration to some form of in-medium cross sections. This addition will be made and the current version should be viewed as an interim developmental step in the complete process.

Because of the reliance of this method on Hamilton-Jacobi theory, Pauli blocking, and fragment coalescence, quantum final state interactions are included a posteriori rather than being a natural consequence of the central theory. Pauli blocking is included such that a particle cannot scatter back into a state with momentum below the Fermi level in its original nucleus. Coalescence is achieved through an again tedious, but necessary calculation of combinatorial possibilities based on proximity with regard to spatial coordinate and momentum, effectively working towards a minimization of “coalescence volume”. Final state interactions are included by allowing further collisions and interactions to occur after the initial set of reactions characteristic of the two nuclei passing through the overlap or “fireball” region. This includes interactions between product pre-fragments.

4. Conclusions

We have succeeded in embedding a heavy ion event generator based on the RQMD approach into the FLUKA Monte-Carlo Transport code. While that event generator has some potential shortcomings, it represents one of the best alternatives for modeling nuclear interactions that occur in collisions of heavy ions at energies from ~ 100 MeV/A up through ~ 5 GeV/A. This effort was motivated principally by NASA’s need to be able to simulate the effects of the exposure of spacecraft and crew members to the space radiation environment. At present, NASA has created a pair of coupled consortia that are charged with developing the kind of event generators that have been discussed here on the one hand, and with making the measurements needed to evaluate the efficacy of those event generators on the other. It is NASA’s intention that these two consortia function in an iterative matter to increase the accuracy of the event generator models to the point where the fluences can be predicted to an accuracy of within 25% from the simulations.

The uses that NASA intends to make of these codes include the direct aiding in the design of the spacecraft and structures that future astronauts will employ in the effort to return to the Moon and to explore Mars. These include the effects of the Martian atmosphere and the Martian and Lunar regoliths as well as for any spacecraft and space suit configurations.

These codes represent the best alternative in the evaluation of the radiation field where complex geometries and mixed elemental materials are concerned. They nicely complement simpler approaches used in estimating this same thing and can act as a validation tool for those calculations as well as for detailed ground and space-based measurements.

The work on these event generators is far from being finished. The greatest need is for accurate data sets over a range of projectile, target and energy values so that the event generators can be improved and ultimately validated. In preparation for these measurements, we are engaged in the development of extensions to the present theoretical approaches to the physics modeling. We are involved in the development of a new HMD event generator that will hopefully be ready for testing as the next round of data becomes available.

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Biography



Larry Pinsky is a Professor of Physics and Chairperson of the Physics Department at the University of Houston. He does research in Relativistic Heavy Ion Physics at CERN in Geneva, Switzerland as part of the ALICE Collaboration. He is a member of NASA's Space Radiation Shielding Program and a P.I. in NASA's Space Radiation Shielding Modeling Consortium. He has done research in experimental elementary particle physics at laboratories in the US such as the Brookhaven National Laboratory, Fermilab and SLAC, and has worked internationally at facilities in Japan and Europe. He has a BS in Physics from Carnegie-Mellon University and an MA and Ph.D. in Physics from the University of Rochester. He also is a licensed attorney and patent attorney with a JD and LLM in Information and Intellectual Property Law from the University of Houston, and he holds a multi-engine instrument flight instructor rating.

